

BIONET

Fragment Libraries

Are you looking for high quality, novel fragments to complement your in-house fragment collections?

Bionet has over 3,534 diverse fragments that are unavailable from other commercial suppliers.

Key Organics has created an enhanced Bionet Fragment Library Ro3. These compounds will greatly appeal to all discovery scientists in the pharma and agrochemistry sectors.



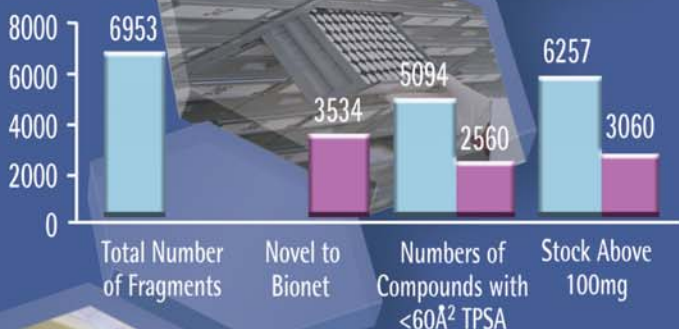
Bionet Fragment Library Ro3 Cluster Analysis

Clustering analysis of the Bionet Fragment Library Ro3 reveals high diversity in the collection. Compounds were fingerprinted with bit-packed MACCS keys⁽¹⁾ and then Jarvis-Patrick clustering was applied with a Tanimoto similarity metric using an 85% threshold for similarity and cluster overlap. The results of this procedure are shown in the table below. There are significant numbers of singletons, illustrating the diversity of the Bionet Fragment Library Ro3 collection.

Rationale

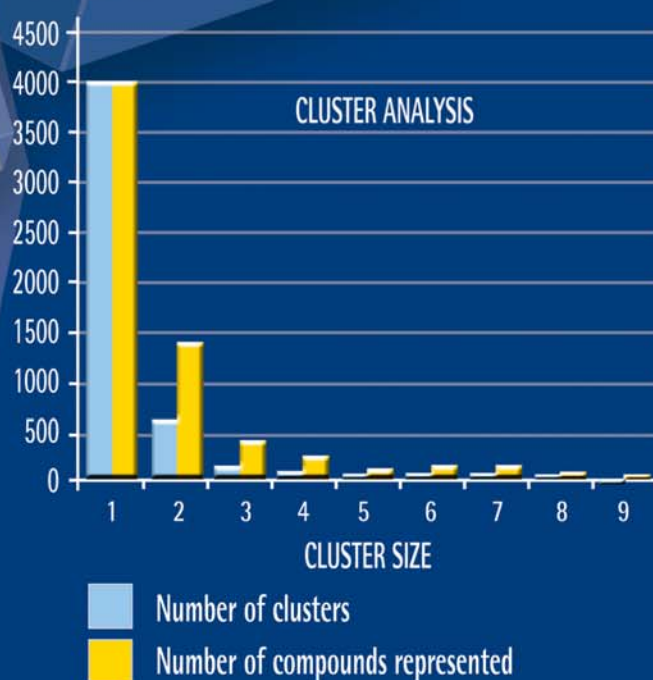
The **Bionet Fragment Library Ro3** encompasses 6,953 carefully selected diverse fragments which have been rigorously chosen for their suitability for fragment based screening applications and further chemical elaboration. It has been established that 3,534 of these fragments are uniquely available through Bionet based on a comparison with commercially available libraries containing >8 million compounds.

All the fragments obey the "Rule of three"⁽¹⁾ and both solubility⁽²⁾ and topological polar surface area (TPSA) descriptors have been calculated.



Pre-plated sets of 500 and 1,000 compounds are available ex-stock for same day dispatch; alternatively customers can cherry pick from the entire fragment collection (currently totalling 6,953 fragments).

(1) Congreve M, Carr R, Murray C, Jhoti H (2003) *Drug Discovery Today* 8, pp876-77
(2) Hou, T.J., Xia, K., Zhang, W., Xu, X.J. (2004) ADME Evaluation in Drug Discovery. 4. Prediction of Aqueous Solubility Based on Atom Contribution Approach *J. Chem. Inf. Comput. Sci.* 44:266-27
(3) Analysis conducted using MOE (Chemical Computing Group Inc.)



Bionet also offers the Bionet Extended Library Set which targets the requirements of fragment optimization. With over 24 years of expertise in providing novel screening compound design and synthesis, Key Organics is well qualified to provide fragment libraries based around any fragment of interest, as well as fragment linkage strategies.

Contact us for solubility/TPSA data and pricing information.

IOCAS ← Key Organics → BIONET

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Key Organics

The right side of the Equation

Key Organics offers a comprehensive range of chemistry solutions to its clients and is a leading global provider in the supply of high quality chemical products and contract services to the pharmaceutical, agrochemical, biotechnology sectors together with related industries and applications.

Key Organics has over 24 years of proven expertise and competence enabling it to become a long-term strategic partner to meet all its clients' chemistry needs. Rather than just selling compounds the primary aim of Key Organics is to provide a consistent, reliable and very high quality service, with unrivalled customer support, technical back-up, guaranteed confidentiality and outstanding performance.

BIONET Products

Under the BIONET brand, Key Organics offer the renowned and extensive 'Bionet Screening', Bionet Intermediates, Bionet Ro3 Fragments, Bionet Assay Standards, Core Scaffolds and Agrimediate™ Collections

KOCAS Services

Tailor-made services under the KOCAS brand include Custom chemistry, Contract/FTE chemistry, Library development, KOCitius, KOSYnergi, and Analytical support services

Whatever the chemistry requirements, Key Organics can be trusted to offer the best value solutions to meet individual needs.

BIONET



Key Organics



KOCAS

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Assay Standards
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Core Scaffolds
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